

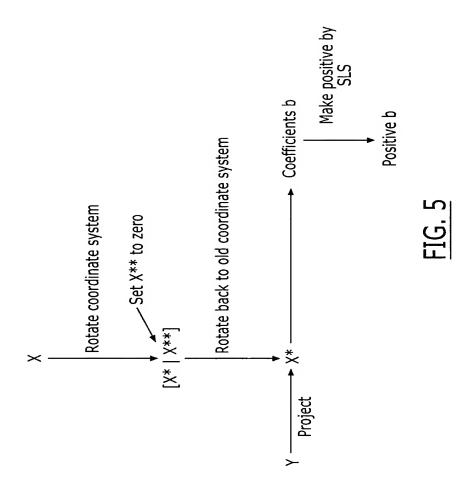
FIG. 3

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The number of columns Generate a mathematical The number of individual design matrix "X" of constituent data in the design matrix can constituent data sets is at least 10, each representing a respective one of at least 10 different closely correlated chemical correspond to the number comprising a plurality of individual mathemof different individual constituents of interest and, where needed, at atical constituent matrix data sets, each constituent data set leást one additional constituents, some of the constituents having column representing including amplitude values of a respective spectrum lineshape of a overlapping signal lines in a region of the spectrum analyzed. spectra contributions from at least one non-relevant variable constituent and/ or noise. 201 selected independent constituent parameter over desired data points generated by a pre-determined analysis The predetermined analysis Generate a composițe method is NMR mathematical matrix "Y" spectroscopy, and the method. 200 comprising a data set of composite signal represents: amplitude values of a intensity over a desired composite spectrum lineshape over the desired interval or region in a Rotate the design matrix chemical shift spectrum to yield a rotated design matrix ("Z") of principal data points for an unknown such that intensity is the sample that is generated by dependent variable the predetermined analysis components and parameter. method, the composite selectively excluding 212 lineshape comprising spectral data for certain principal contributions from a plurality components to generate Compute <u>a</u> normal equations a reduced design of the selected individual matrix (" X^TX ") from the design matrix (X*). constituents. matrix("X). 225 205 Use a sequential least squares statistical Compute regression fit weighting coefficients based regression analysis to restrain negative cóefficients on accepted principal components of the rotated design matrix ("Z") in the reduced design matrix (X*) to zero unțil all constituents of interest are non-negative. to determine the presence of and/or measurement of the selected constituents. 230 Interrogate the normal equations matrix ("X1X")

FIG. 4

by applying a predetermined acceptance function (A) to the principal components.



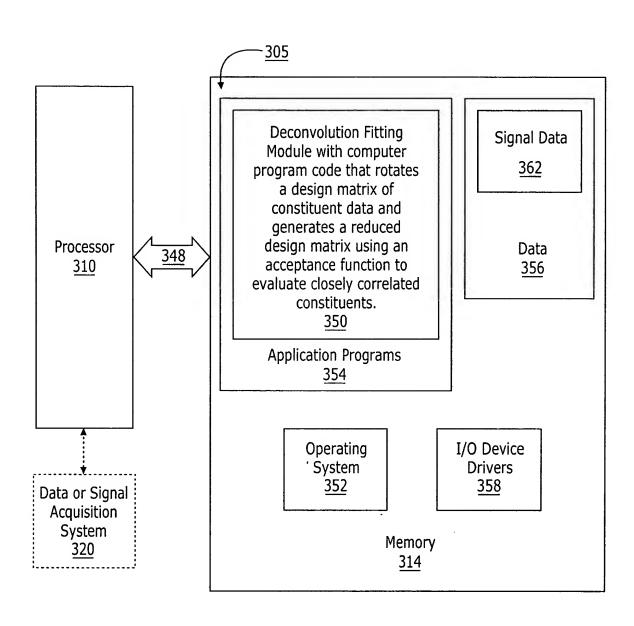


FIG. 6

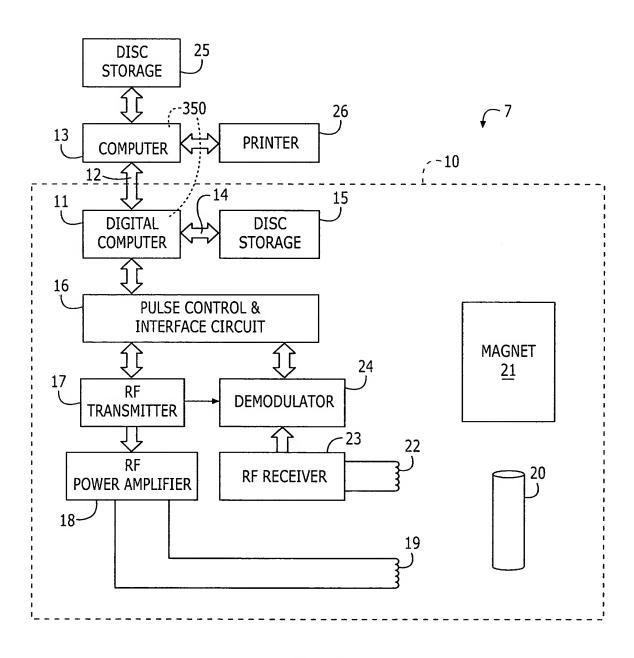


FIG. 7

